

Vertical balance equations

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Last update: May 9, 2025

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1 Block formulation

Let $\mathbf{x} \in \mathbb{R}^n$ be the “balanced variable” and $\mathbf{v} \in \mathbb{R}^n$ be the “unbalanced variable”. They are linked through a “balance operator” $\mathbf{K} \in \mathbb{R}^{n \times n}$:

$$\mathbf{x} = \mathbf{K}\mathbf{v} \quad (1)$$

Let split \mathbf{x} and \mathbf{v} into m blocks, and \mathbf{K} into m^2 square blocks:

$$\begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{pmatrix} = \begin{pmatrix} \mathbf{K}_{1,1} & \cdots & \mathbf{K}_{1,m} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{m,1} & \cdots & \mathbf{K}_{m,m} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_m \end{pmatrix} \quad (2)$$

or

$$\mathbf{x}_i = \sum_{j=1}^m \mathbf{K}_{i,j} \mathbf{v}_j \quad (3)$$

where the size of each sub-vector \mathbf{x}_i and \mathbf{v}_i is n_i , with $\sum_{i=1}^m n_i = n$, and $\mathbf{K}_{i,j} \in \mathbb{R}^{n_i \times n_j}$.

2 Triangular assumption

We assume that the balance operator \mathbf{K} is block-lower-triangular, with identity diagonal blocks:

$$\mathbf{K} = \begin{pmatrix} \mathbf{I}_n & 0 & \cdots & \cdots & 0 \\ \mathbf{K}_{2,1} & \mathbf{I}_n & \ddots & & \vdots \\ \mathbf{K}_{3,1} & \mathbf{K}_{3,2} & \mathbf{I}_n & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \mathbf{K}_{m,1} & \mathbf{K}_{m,2} & \cdots & \mathbf{K}_{m,m-1} & \mathbf{I}_n \end{pmatrix} \quad (4)$$

Thus, we can simplify equation (3) into:

$$\mathbf{x}_i = \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j + \mathbf{v}_i \quad (5)$$

3 Adjoint

The adjoint of the balance operator is given by:

$$\mathbf{K}^T = \begin{pmatrix} \mathbf{I}_n & \mathbf{K}_{2,1}^T & \mathbf{K}_{3,1}^T & \cdots & \mathbf{K}_{m,1}^T \\ 0 & \mathbf{I}_n & \mathbf{K}_{3,2}^T & \cdots & \mathbf{K}_{m,2}^T \\ \vdots & \ddots & \mathbf{I}_n & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \mathbf{K}_{m,m-1}^T \\ 0 & \cdots & \cdots & 0 & \mathbf{I}_n \end{pmatrix} \quad (6)$$

so $\mathbf{v} = \mathbf{K}^T \mathbf{x}$ can be expressed as:

$$\mathbf{v}_i = \mathbf{x}_i + \sum_{j=i+1}^m \mathbf{K}_{j,i}^T \mathbf{x}_j \quad (7)$$

4 Partial recursive inverse

Equation (5) can be transformed to compute \mathbf{v} knowing \mathbf{x} recursively:

$$\mathbf{v}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \quad (8)$$

It should be noted that the inverse of $\mathbf{K}_{i,j}$ is not required. This inverse formula is referred to as “partial” since the unbalanced variable \mathbf{v} still appears on the right-hand side.

For the adjoint in equation (7), the same transformation leads to:

$$\mathbf{x}_i = \mathbf{v}_i - \sum_{j=i+1}^m \mathbf{K}_{j,i}^T \mathbf{x}_j \quad (9)$$

and must be applied recursively in reverse order (i from m to 1).

5 Full recursive inverse

We assume that for $1 \leq j \leq i$, there are matrices $\mathbf{A}_{i,j} \in \mathbb{R}^{n_i \times n_j}$ such that \mathbf{v}_i can be expressed as:

$$\mathbf{v}_i = \sum_{j=1}^i \mathbf{A}_{i,j} \mathbf{x}_j \quad (10)$$

Plugging this expression into the partial recursive inverse formula (8), we get:

$$\begin{aligned} \mathbf{v}_i &= \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \\ &= \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \sum_{k=1}^j \mathbf{A}_{j,k} \mathbf{x}_k \\ &= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=1}^j \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\ &= \mathbf{x}_i - \sum_{k=1}^{i-1} \sum_{j=k}^{i-1} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\ &= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \mathbf{x}_j \end{aligned} \quad (11)$$

Thus, using this result and equation (10) again, we get:

$$\mathbf{v}_i = \sum_{j=1}^i \mathbf{A}_{i,j} \mathbf{x}_j = \sum_{j=1}^{i-1} \left(- \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \right) \mathbf{x}_j + \mathbf{x}_i \quad (12)$$

which is verified if:

$$\mathbf{A}_{i,i} = \mathbf{I}_n \quad (13a)$$

$$\mathbf{A}_{i,j} = - \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \quad (13b)$$

6 Statistical property

Since \mathbf{v} is an “unbalanced variable”, it has the following statistical property:

$$\text{if } i \neq j, \text{ Cov}(\mathbf{v}_i, \mathbf{v}_j) = 0 \quad (14)$$

7 Estimation with the partial recursive inverse

Using the partial recursive inverse (8) for $j < i$, we get:

$$\text{Cov}(\mathbf{v}_j, \mathbf{v}_i) = 0 \quad (15)$$

$$\Leftrightarrow \text{Cov} \left(\mathbf{v}_j, \mathbf{x}_i - \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \mathbf{v}_k \right) = 0 \quad (16)$$

$$\Leftrightarrow \text{Cov}(\mathbf{v}_j, \mathbf{x}_i) = \text{Cov} \left(\mathbf{v}_j, \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \mathbf{v}_k \right) \quad (17)$$

$$= \sum_{k=1}^{i-1} \text{Cov}(\mathbf{v}_j, \mathbf{v}_k) \mathbf{K}_{i,k}^T \quad (18)$$

Using the statistical property (14) of \mathbf{v} , the term for which $k = j$ is the only one remaining in the right-hand side:

$$\begin{aligned} \text{Cov}(\mathbf{v}_j, \mathbf{x}_i) &= \text{Cov}(\mathbf{v}_j, \mathbf{v}_j) \mathbf{K}_{i,j}^T \\ \Leftrightarrow \text{Cov}(\mathbf{x}_i, \mathbf{v}_j) &= \mathbf{K}_{i,j} \text{Cov}(\mathbf{v}_j, \mathbf{v}_j) \\ \Leftrightarrow \mathbf{K}_{i,j} &= \text{Cov}(\mathbf{x}_i, \mathbf{v}_j) \text{Cov}(\mathbf{v}_j, \mathbf{v}_j)^{-1} \end{aligned} \quad (19)$$

8 Expression with the full recursive inverse

Using the full recursive inverse (10), we get for $j < i$:

$$\begin{aligned}\text{Cov}(\mathbf{x}_i, \mathbf{v}_j) &= \text{Cov}\left(\mathbf{x}_i, \sum_{k=1}^j \mathbf{A}_{j,k} \mathbf{x}_k\right) \\ &= \sum_{k=1}^j \text{Cov}(\mathbf{x}_i, \mathbf{x}_k) \mathbf{A}_{j,k}^T\end{aligned}\quad (20a)$$

$$\begin{aligned}\text{Cov}(\mathbf{v}_j, \mathbf{v}_j) &= \text{Cov}\left(\sum_{k=1}^j \mathbf{A}_{j,k} \mathbf{x}_k, \sum_{l=1}^j \mathbf{A}_{j,l} \mathbf{x}_l\right) \\ &= \sum_{k=1}^j \mathbf{A}_{j,k} \sum_{l=1}^j \text{Cov}(\mathbf{x}_k, \mathbf{x}_l) \mathbf{A}_{j,l}^T\end{aligned}\quad (20b)$$

which allows a computation of the balance operator $\mathbf{K}_{i,j}$ using expression (19).

9 Practical computations

In practice, covariances are sampled from an ensemble. Let $\{\tilde{\mathbf{x}}^1, \dots, \tilde{\mathbf{x}}^N\}$ be a set of N vectors that samples the distribution of \mathbf{x} and $\{\delta\tilde{\mathbf{x}}^1, \dots, \delta\tilde{\mathbf{x}}^N\}$ their centered counterparts:

$$\delta\tilde{\mathbf{x}}^p = \tilde{\mathbf{x}}^p - \langle \tilde{\mathbf{x}} \rangle \quad (21)$$

where $\langle \cdot \rangle$ denotes the ensemble mean:

$$\langle \tilde{\mathbf{x}} \rangle = \frac{1}{N} \sum_{p=1}^N \tilde{\mathbf{x}}^p \quad (22)$$

The covariance $\text{Cov}(\mathbf{x}_i, \mathbf{x}_j)$ can be estimated from these perturbations by:

$$\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{N-1} \sum_{p=1}^N \delta\tilde{\mathbf{x}}_i^p (\delta\tilde{\mathbf{x}}_j^p)^T \quad (23)$$

Because of the limited ensemble size N , it can be relevant to filter the covariance matrix with a linear operator \mathcal{F} :

$$\overline{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) = \mathcal{F} \left[\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) \right] \quad (24)$$

The algorithm to compute the balance operator components using the partial recursive inverse equation (8) is detailed in algorithm 1. Its counterpart using the full recursive inverse equation (10) is detailed in algorithm 2. It should be noted that:

- The first method requires storing the ensemble twice, while the second requires storing more matrices.
- When a filtering \mathcal{F} is applied, both methods can yield different results but there is no theoretical way to know which one is the most accurate.

Algorithm 1 Recursive computation of the balance operator components using the partial recursive inverse formula

Copy the ensemble perturbations:

for $1 \leq p \leq N$ **do**

$$\delta \widetilde{\mathbf{v}}^p = \delta \widetilde{\mathbf{x}}^p$$

end for

for $1 \leq i \leq m$ **do**

for $1 \leq j < i$ **do**

Estimate the cross-covariance between \mathbf{x}_i and \mathbf{v}_j :

$$\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) = \frac{1}{N-1} \sum_{p=1}^N \delta \widetilde{\mathbf{x}}_i^p (\delta \widetilde{\mathbf{v}}_j^p)^T$$

Filter the cross-covariance between \mathbf{x}_i and \mathbf{v}_j :

$$\overline{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) = \mathcal{F} \left[\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) \right]$$

Inverse $\overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)$ to get $\overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)^{-1}$

Compute the balance operator component $\mathbf{K}_{i,j}$:

$$\mathbf{K}_{i,j} = \overline{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) \overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)^{-1}$$

Update the unbalanced ensemble perturbations:

for $1 \leq p \leq N$ **do**

$$\delta \widetilde{\mathbf{v}}_i^p \leftarrow \delta \widetilde{\mathbf{v}}_i^p - \mathbf{K}_{i,j} \delta \widetilde{\mathbf{v}}_j^p$$

end for

end for

if $i < m$ **then**

Estimate the auto-covariance of \mathbf{v}_i :

$$\widetilde{\text{Cov}}(\mathbf{v}_i, \mathbf{v}_i) = \frac{1}{N-1} \sum_{p=1}^N \delta \widetilde{\mathbf{v}}_i^p (\delta \widetilde{\mathbf{v}}_i^p)^T$$

Filter the auto-covariance of \mathbf{v}_i :

$$\overline{\text{Cov}}(\mathbf{v}_i, \mathbf{v}_i) = \mathcal{F} \left[\widetilde{\text{Cov}}(\mathbf{v}_i, \mathbf{v}_i) \right]$$

end if

end for

Algorithm 2 Recursive computation of the balance operator components using the full recursive inverse formula

for $1 \leq i \leq m$ **do**

for $1 \leq j \leq i$ **do**

 Estimate the cross-covariance between \mathbf{x}_i and \mathbf{x}_j :

$$\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{N-1} \sum_{p=1}^N \delta \widetilde{\mathbf{x}}_i^p \left(\delta \widetilde{\mathbf{x}}_j^p \right)^T$$

 Filter the cross-covariance between \mathbf{x}_i and \mathbf{x}_j :

$$\overline{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) = \mathcal{F} \left[\widetilde{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j) \right]$$

end for

end for

for $1 \leq i \leq m$ **do**

for $1 \leq j < i$ **do**

 Compute the cross-covariance between \mathbf{x}_i and \mathbf{v}_j :

$$\overline{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) = \sum_{k=1}^{j-1} \overline{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_k) \mathbf{A}_{j,k}^T + \overline{\text{Cov}}(\mathbf{x}_i, \mathbf{x}_j)$$

 Inverse $\overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)$ to get $\overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)^{-1}$

 Compute the balance operator component $\mathbf{K}_{i,j}$:

$$\mathbf{K}_{i,j} = \overline{\text{Cov}}(\mathbf{x}_i, \mathbf{v}_j) \overline{\text{Cov}}(\mathbf{v}_j, \mathbf{v}_j)^{-1}$$

end for

for $1 \leq j < i$ **do**

 Compute the matrix $\mathbf{A}_{i,j}$:

$$\mathbf{A}_{i,j} = - \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \overline{\mathbf{A}}_{k,j}$$

end for

if $i < m$ **then**

 Compute temporary matrices $\mathbf{S}_{k,i}$:

for $1 \leq k \leq i$ **do**

$$\mathbf{S}_{k,i} = \sum_{l=1}^k \overline{\text{Cov}}(\mathbf{x}_k, \mathbf{x}_l) \mathbf{A}_{i,l}^T + \sum_{l=k+1}^{i-1} \overline{\text{Cov}}(\mathbf{x}_l, \mathbf{x}_k)^T \mathbf{A}_{i,l}^T + \overline{\text{Cov}}(\mathbf{x}_k, \mathbf{x}_i)$$

end for

 Compute the auto-covariance of \mathbf{v}_i :

$$\overline{\text{Cov}}(\mathbf{v}_i, \mathbf{v}_i) = \sum_{k=1}^{i-1} \mathbf{A}_{i,k} \mathbf{S}_{k,i} + \mathbf{S}_{i,i}$$

end if

end for
